

Oxazole  
288-42-6 | DTXSID70182983

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.91            | 1.08 | 0.91           | 1.08 | 0.92       | 1.00 |

Model Results

Predicted value: 99.5 mmHg

Global applicability domain: Inside

Local applicability domain index: 6.65e-01

Confidence level: 8.45e-01

Nearest Neighbors from the Training Set

|   |   |   |
|---|---|---|
| <div>Image not found</div> <div>4-Methyl-1-pentene</div> <div>Measured: 313</div> <div>Predicted: 268</div>   | <div>Image not found</div> <div>4-Methoxy-4-methyl-2-pentanone</div> <div>Measured: 90.2</div> <div>Predicted: 6.05</div> | <div>Image not found</div> <div>3-Chloro-1,2-propanediol</div> <div>Measured: 86.6</div> <div>Predicted: 1.74e-01</div> |
| <div>Image not found</div> <div>Methacrylamide</div> <div>Measured: 38.5</div> <div>Predicted: 4.66e-02</div> | <div>Image not found</div> <div>Ethylene glycol dimethyl ether</div> <div>Measured: 82.6</div> <div>Predicted: 86.5</div> |   |